# Simulations of mid infrared emission of InAsN semiconductors

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# Simulations of Mid Infrared Emission of Dilute Nitride Semiconductors

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**Abstract:** This paper delivers an efficient approximation to the complex many body problem of luminescence in semiconductors to the case of mid infrared luminescence of dilute nitrides. The results are in good agreement with recent experimental data.

## 1. Introduction

Luminescence, absorption and transmission spectra play a major role in the characterization of new materials and optoelectronic devices operating from the THz to the UV ranges [1-7] In this paper we apply an accurate analytical approximation for luminescence that can be easily programmed and includes the main many body effects required to describe bulk semiconductors. The luminescence is connected to the nonlinear absorption and gain and the expressions delivered reduce exactly to Elliott's formula in the low density limit. This leads to an efficient numerical tool to investigate new materials, starting e.g. from ab initio calculations and has potentials for a major impact in the development of new bulk materials for efficient solar cells and for mid infrared radiation generation and detection. The good agreement between the theory and experimental data for mid infrared emitting dilute nitride structures [3] clearly demonstrates the power and accuracy of the approach.

## 2. Mathematical Approach and Model Equations

The optical response of semiconductor materials can be obtained by self-consistent evaluation of Manybody Nonequilibrium Green's Functions (NEGF). Efficient numerical methods used here have been successfully applied to both intersubband [8-14] and interband transitions [15-17] in quantum wells and superlattices. This paper starts from a similar approach that can also describe superlattices as effective 3D anisotropic media [18, 19] and leads to very accurate approximations. We start with the isotropic limit of the interband polarization in an effective anisotropic 3D material [18]. Only diagonal dephasing is used and the population difference factor is given by $A(\omega) = tanh\left(\beta\left(\hbar\omega - \mu\right)/2\right)$, where is $\mu = E_g + \mu_e + \mu_h$ which can be estimated with an analytical approximation [18]. The typical Yukawa potential used to represent the screened Coulomb potential does not have simple analytical solutions. We thus replace it with the Hulthén potential [18]. We use an analytical average for the dephasing $\Gamma$ that partially simulates the electron-electron, electron-phonon and electron-impurity scattering [20-22], which would be required for increased predictability

and are being included in the approach for dilute nitrides.

The choice of inversion factor further guarantees that the cross-over from absorption to gain takes place exactly at the total chemical potential, which allows an application of the Kubo-Martin-Schwinger (KMS) relation [15,23-24] to deliver an analytical expression for the optical photoluminescence spectra $L(\omega)$, valid under linear and nonlinear excitation conditions such as in nonlinear pump and probe luminescence experiments [15, 25].

$$L(\omega) = L_0 \left(\frac{\hbar\omega}{E_0}\right)^3 \frac{1}{e^{\beta(\hbar\omega-\mu)}+1} \left\{ \sum_{n=1}^{g^{1/2}} \frac{4\pi}{n}\left(\frac{1}{n^2}-\frac{n^2}{g^2}\right)\delta_\Gamma\left(\Delta-\frac{E_n}{E_0}\right) + 2\pi\int_0^\infty dx \frac{sinh\pi g\sqrt{x}}{cosh\pi g\sqrt{x}-cosh\pi\sqrt{xg^2-4g}}\delta_\Gamma(\Delta-x)\right\}. \quad (1)$$

In equation (1) above, the first term is the excitonic luminescence which dominates the entire process at low temperatures, while the second term is the contribution from the continuum where the excitons have ionized. The bound states are given by $E_n = -E_0\left(n^{-1}-ng^{-1}\right)^2$. Furthermore, $L_0 = 2|\wp|^2 E_0^2 n_b/(\pi^2\hbar^3c^3a_0^3)$ and the normalized detuning is $\Delta(\omega) = (\hbar\omega - E_g)/E_0$. The symbols $n_b$ and c denote, respectively, the background refractive index and the speed of light in vacuum. The 3D exciton binding energy and radius are given by $E_0$ and $a_0$. $\wp$ is the transition dipole moment.

In equation (1) above, the band gap renormalization stems from the Mott criterion. This choice of bandgap renormalization is usually in good agreement with the full Green's function approach and the single Plasmon pole approximation (SPPA) simplified under a quasistatic approximation [18].

$$E_g = E_{g0} + E_0 \begin{cases} -1+(1-1/g)^2, & g \geq 1 \\ -1/g, & g < 1 \end{cases} \quad (2)$$

where $g = 1/\kappa a_0$ is the screening length is given by the relation $\kappa^2 = \frac{4\pi e^2}{\grave{o}_0}\sum_i \frac{\partial n_i}{\partial \mu_i}$. $n_i$ denotes the number of electrons or holes and $E_{g0}$ is the conventional (temperature dependent) isotropic bandgap. The broadened delta function is chosen as $\delta_\Gamma(x) = 1/\pi\Gamma cosh(x/\Gamma)$, which reproduces the Urbach tail very efficiently. The sum in the exciton part runs through the available states within the largest integer value of $\sqrt{g}$. In the low density limit $g \to \infty$ and we recover the Elliot formula for excitonic luminescence with the correct balance between bound and continuum states.

## 3. Numerical Results and Discussion

Figure 1 shows calculated luminescence spectra at low power level compared with experimental data. The bandgap stems from the BAC Model

$$E_{\pm}(k) = \frac{1}{2}\left\{[E_k^C + E^N] \pm \sqrt{[E_k^C - E^N]^2 + 4V^2x}\right\}. \quad (3)$$

Here $E_c(k)$ is the conduction band dispersion of the unperturbed non-nitride semiconductor taken at $k = 0$, i.e the band gap. $E_N$ is the position of the nitrogen impurity level, $V_{CN}$ is the interaction potential and $x$ is the nitrogen composition. For dilute nitride $InAs_{1-x}N_x$, the following values can be taken for the parameters $V = 2.0eV$ [3] and the position of the Nitrogen impurity, $E^N = 1.44eV$ [26-27]. The temperature dependent band gap of the host matrix (InAs) follows the Varshni formula [28-30];

$$E_{gInAs} = 0.415 - \left((2.76\text{x}10^{-4})\frac{\text{T}^2}{\text{T}+93}\right). \quad (4)$$

It is noteworthy that the CB band anti-crossing model is only valid at a very small nitrogen composition $x \leq 0.03$. The band gap obtained for the BAC model is consistent with the recommended band gap law for N- containing semiconductors with bowing parameter, $b = 4.22eV$ [28].

$$E_{g[InAs_{1-x}N_x]} = (E_{g[InN]})x + (1-x)E_{g[InAs]} - bx(1-x). \quad (5)$$

The difference in linewidth can be attributed to inhomogenous broadening that arises from a fluctuation in N-concentration and can also be described by our approach, but this requires a phenomenological broadening factor for the N-distribution that even though leads to a better agreement with experiments, reduces the impact of the microscopic formulas and is thus not shown here. The inhomogeneous broadening typically shifts the spectral peak as well.

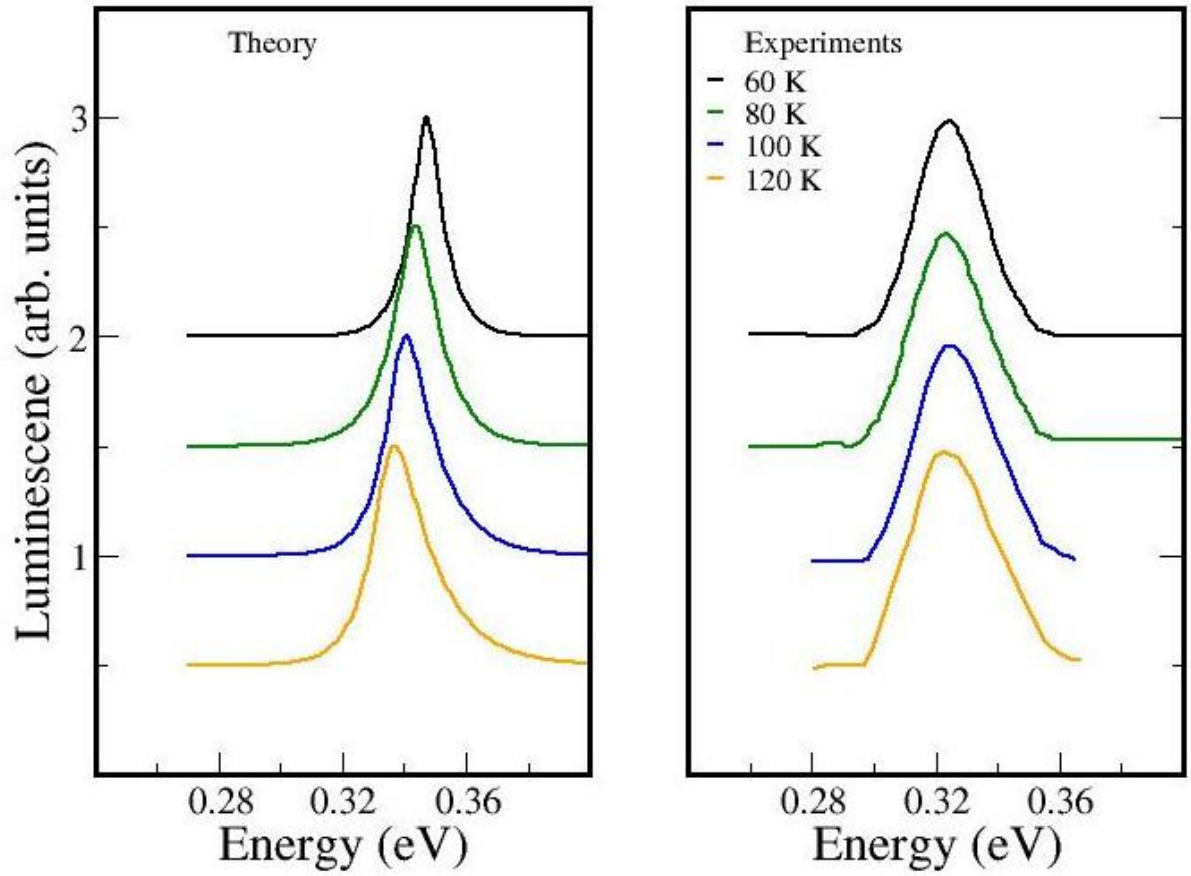


*Fig.1. Theoretical (left) vs Experimental (right) luminescence for a InAsN sample at various temperatures. The experimental data for comparison has been extracted from [3] Krier et al. The experiments show broader lines due to inhomogeneous broadening, which is not included in the simulations to keep the reference results as microscopic as possible. It also typically shifts the spectral peak. Inhomogeneous broadening would require the use of a fit phenomenological parameter. The density used in the calculations is* $N=10^{14}$ *carriers/cm*$^3$.

## 4. Conclusion

In conclusion, we have presented a simple and accurate expression for the optical luminescence of semiconductors materials, valid in both linear and nonlinear regimes, i.e. for an arbitrary density of carriers. In contrast to previous materials found in the literature, the corresponding optical absorption reduces exactly to Elliott's formula for excitons at low density with the correct balance between bound and continuum states. The bulk InAsN structure, which is relevant for Mid Infrared applications and chosen for numerical examples, illustrates the power of the method to study new materials, whose band structure can be obtained from ab initio calculations. The expressions delivered can be applied for the characterization of new materials and efficient designs of devices based on them and have potential for a huge impact on both basic science and technological applications.

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